

MODELING AND DESIGN SYSTEMS FOR INTEGRATED MICROELECTROMECHANICAL DEVICES

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What I'd like to talk about today is some of the problems that we see in mechanical behavior on the micron scale. While the data presented is from micro electro mechanical systems (MEMS), the behavior is, in some respects, similar to what occurs in seals. We'll show some model results and compare the model predictions to experimental results and see where we're successful and where we still have flaws in our understanding of the physics of mechanical behavior at the micron level. In table 1, I have listed some of the critical modeling issues in MEMS.

Unique modeling requirements of MEMS

Large range of Dimensions
Coupled fields
Large gradients in solutions

Table 1.

If I got rid of the title micro electro mechanical system (MEMS) and retitled the table critical modeling issues in seals you probably use the same slide. In MEMS, we have large ranges of dimensions their awfully small but we're talking about three to four quarters magnitude differences in dimensions between flow fields in the narrow regions and flow fields in the bulk region. Both MEMS and seals have large gradients in fields; things happen over very small regions. This is something that seems to have plagued most of the numerical schemes; the ability to capture those small regions without killing the possibility of solutions of the bulk region. Most of the problems involve some sort of coupling between different fields. In a turbine seals we're concerned about the interaction between rotor dynamics, the deformation of small flexible surfaces that comprise the seal, also the fluid flow and some thermal problems. In the case of MEMS devices we have an interest thermal problems, fluid mechanics, the solid mechanic components, and also electric fields that are used as part of driving mechanism too, so lots of similarity.

Meteorites don't fall on the earth. They fall on the Sun - and the Earth gets in the way – John W. Campbell

I sort of like this quotation and I use it every once in awhile. what you really have to remember when examining mechanical behavior on the micron scale is that some of the expected behavior of bulk materials does not apply to devices on this scale. When you talk about modeling micro devices, a lot of our conventional thinking about continuum mechanics start to break down. If one thinks of the size of a mechanics problem, in large enough problems, one often treats solid bodies as particles. For

example, planetary motions. If one is modeling the motion of a meteorite heading towards the earth, one very rarely concerns themselves about the elastic vibrations (continuum model) of the meteorite. One is more concerned about what the trajectory is and where the meteorite is going to hit. If one looks at a smaller scale, not necessarily micro but conventional scale, what we turn to, to model devices is continuum mechanics. If you get small enough in the solid mechanics systems you no longer can treat the material as continuum and surprisingly that division doesn't necessarily have to take place on the atomic scale.

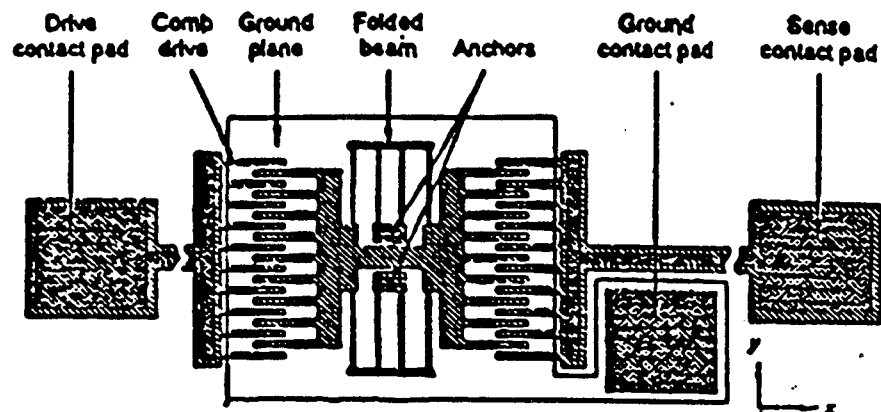
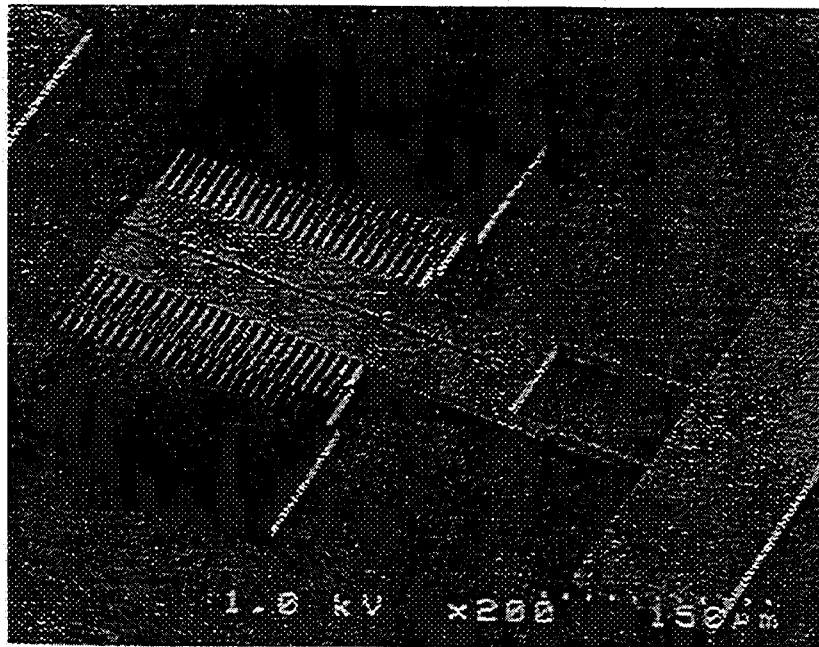
Figure 1 shows a micro materials testing device or fracture mechanics machine. The dimensions are a hundred fifty microns across. The way the device operates is we pre-notched a sample (A) here. D are electrically statically driven elements that have huge surface areas so you can develop reasonably large static forces, reasonable large in this case being a hundred micro-Newtons but its reasonable enough to cause motion on this scale. A, the center section, is raised off the substrate and our interest is in fracture toughness of this device. The fracture mechanics we start with are based on continuum theories. The results from our testing show a fracture toughness (J_c) of about 25 N/m for polysilicon on the micron scale. Values reported for silicon bulk fracture toughness are around 5 N/m. In addition we see a larger scatter in our smaller devices than is reported for bulk materials. One of the things we decide to do is just look and see can we use a continuum model for this scenario. One of concerns here is if you look at a micro graph especially the after fracture the polysilicon is a polycrystalline material and the crystals size in a typical low pressure CVD film are between one half a micron and a micron in size. The uncracked ligament in the fracture device is on the order of five to ten grains of volume. In seals if look at a thin coating, one can again see a material that is composed of a small number of grains.

In order to model the behavior of a material that is not a single crystal (anisotropic homogeneous) and not composed of a large number of crystals (isotropic homogeneous) we used a Monte-Carlo simulation using distributions of single crystals (anisotropic heterogeneous) using finite elements. For the thin film fracture device, we treat as two dimensional plain strain because micrographs show that the structure of the film is column like in the thickness direction. We have columnar growth. In the plane of polycrystalline formulation nucleation sites are assumed random and we assume a crystal growth until it hits another boundary. With those assumptions you're going to end up with Poisson distribution for the number of crystal in a particular volume and end up with a topology that sort of looks like a Voronoi-cell distribution composed of polygons, figure 2.

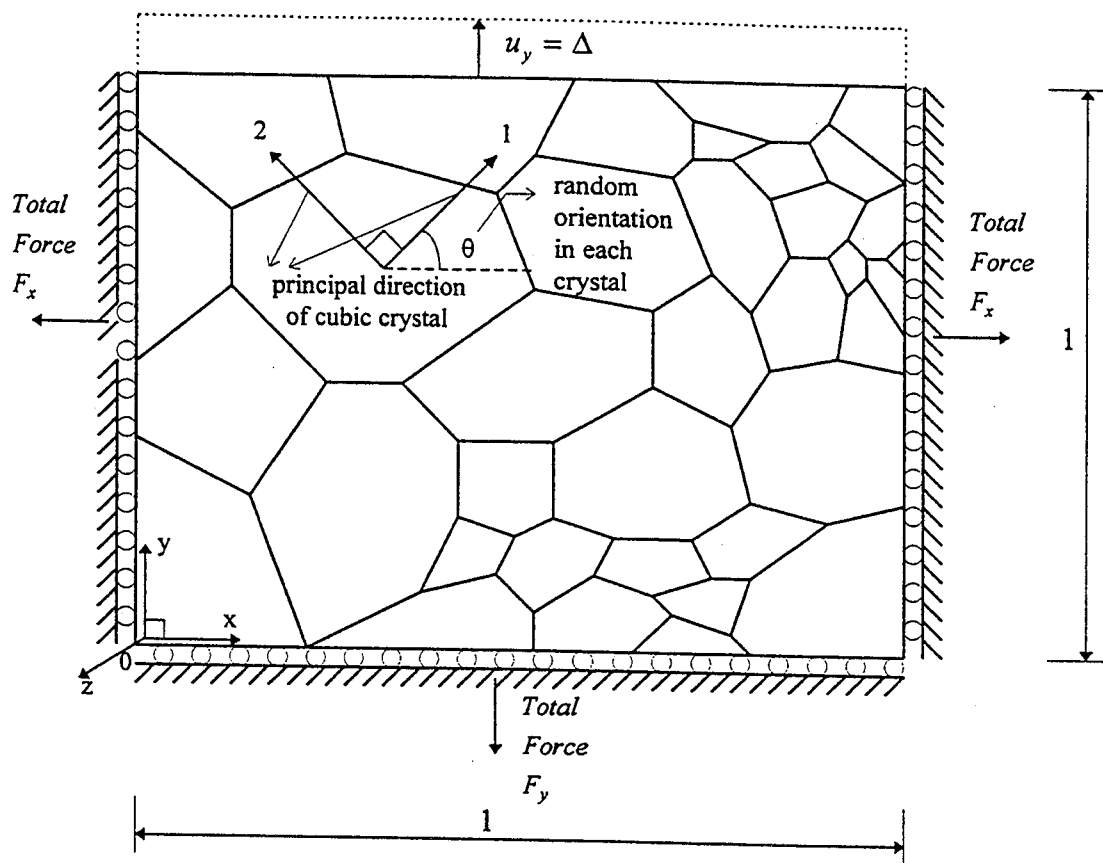
Every intersection or vertex has three polygons or three lines coming in except for the corners where we have truncated the domain. So we constructed a number of realizations and solved for the apparent properties of the collection of grains. Figure 3 is a plot showing the realizations for the Young's modulus each dot representing a particular realization for the Monte Carlo simulation of unit cube containing ten up to a thousand crystals. The reported bulk value for Young's modulus for polysilicon is

about 1.6 Gpa. From the figure one can see fairly significant variation in the modulus in the region where you have between ten and a hundred grains. If you're trying to predict properties here you have to expect that the best you're going to be able to if all the processing steps are identical is a modulus with a ten percent variation. So when you design those sort of systems you have to take that into consideration.

We're going to look at a couple examples of fluid mechanics. Again, we're going to see ranges where we're unable to predict the fluid mechanics response correctly because the dimension is getting small in terms of the mean free path of the fluid. In this particular problem a top plate is moved towards a bottom surface. There is a continuing variation in the geometry as the top plate starts coming down. The initial separation is ten microns and the final spacing is a half micron. Figure 4 shows the measured and calculated (by three dimensional Navier Stokes finite element modeling). One can see where the Navier Stokes solution deviate from the measured behavior. I'm very suspect of that fact that we keep hitting below the continuum level in fluid flow and need a transition between continuum and molecular dynamics models to simulate the behavior of these devices. With that I'll close and take any questions.



Layout of lateral resonant device



Poisson-Voronoi Tessellation of
Microstructure for n -grains ($n=5-1000$)

